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enhanced
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NEWS
      16 APR 28
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      17 MAY 23
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      18 MAY 23
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     Trypsin-specific acyl-4-quanidinophenyl esters for
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     bond formation
ΑU
     Gunther, Robert; Thust, Sven; Hofmann, Hans-Jorg; Bordusa, Frank
     Department of Biochemistry, Faculty of Biosciences, Pharmacy and
CS
     Psychology, University of Leipzig, Halle/Saale, Germany
SO
     European Journal of Biochemistry (2000), 267(12), 3496-3501
     CODEN: EJBCAI; ISSN: 0014-2956
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LA
     English
AB
     The function of acyl-4-guanidinophenyl esters as substrate
mimetics for
     the serine protease \alpha-chymotrypsin was investigated by
     protein-ligand docking, hydrolysis, and acyl transfer expts.
the basis
     of protein-ligand docking studies, the binding and hydrolysis
properties
     of these artificial substrates were estimated. The predictions
of the rational
     approach were confirmed by steady-state hydrolysis studies on
     4-guanidinophenyl esters derived from coded amino acids (which
     \alpha-chymotrypsin is not specific for), non-coded amino acids, and
even
     simple carboxylic acid moieties. Enzymic peptide syntheses
qualify these
     esters as suitable acyl donors for the coupling of acyl
components far
     from the natural enzyme specificity, thus considerably expanding
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the

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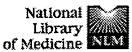
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Theoretical perspectives on the reaction mechanism of serine proteases: the reaction free energy profiles of the acylation process.

J Am Chem Soc. 2003 Oct 1;125(39):12035-48. PMID: 14505425 [PubMed - indexed for MEDLINE]







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L4	0	l1 near10 l2	USPAT	OR	OFF	2005/08/01 11:41
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L6	19	(isoleucine near3 "212") or I217 or Ile217	USPAT	OR	OFF	2005/08/01 11:58
L7	0	l1 near29 l6	USPAT	OR	OFF	2005/08/01 11:58